

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 120 °C

Global applicability domain: Inside

Local applicability domain index: 7.64e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Secbumeton</div> <div>Measured: 87.0</div> <div>Predicted: 112</div>	<div>Image not found</div> <div>Prometon</div> <div>Measured: 91.5</div> <div>Predicted: 112</div>	<div>Image not found</div> <div>Terbumeton</div> <div>Measured: 124</div> <div>Predicted: 117</div>
<div>Image not found</div> <div>Atrazine</div> <div>Measured: 173</div> <div>Predicted: 187</div>	<div>Image not found</div> <div>Propazine</div> <div>Measured: 213</div> <div>Predicted: 197</div>	